



Full wwPDB EM Validation Report ⓘ

Jul 16, 2025 – 02:21 AM JST

PDB ID : 9IZ0 / pdb_00009iz0
EMDB ID : EMD-61006
Title : ATM/Tel1 bound to CHK2 peptide
Authors : Wang, P.
Deposited on : 2024-07-31
Resolution : 3.63 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

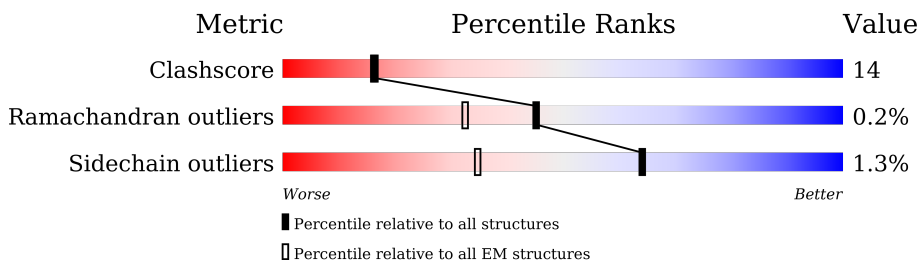
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.63 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	F	8	<div> <div style="width: 62%; background-color: green;"></div> <div style="width: 38%; background-color: yellow;"></div> </div> <div>62% 38%</div>
2	A	2812	<div> <div style="width: 68%; background-color: green;"></div> <div style="width: 18%; background-color: yellow;"></div> <div style="width: 14%; background-color: grey;"></div> </div> <div>68% 18% 14%</div>
2	B	2812	<div> <div style="width: 68%; background-color: green;"></div> <div style="width: 18%; background-color: yellow;"></div> <div style="width: 14%; background-color: grey;"></div> </div> <div>68% 18% 14%</div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 32048 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

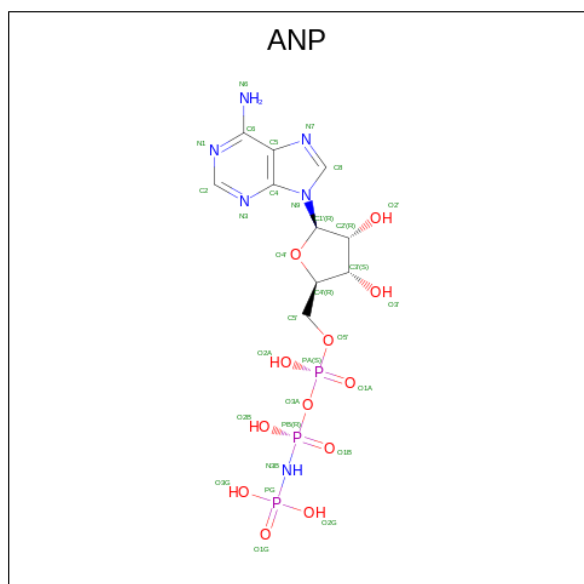
- Molecule 1 is a protein called VAL-SER-THR-GLN-GLU-LEU-TYR-SER.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	F	8	Total	C	N	O	0	0
			64	40	9	15		

- Molecule 2 is a protein called Serine/threonine-protein kinase tel1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	2430	Total	C	N	O	S	0	0
			15929	10030	2839	3040	20		
2	B	2424	Total	C	N	O	S	0	0
			15993	10091	2847	3035	20		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	6	12	3	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	B	1	31	10	6	12	3	0

- Molecule 2: Serine/threonine-protein kinase tel1

Response	Percentage
U.S. should take action to protect the environment	68%
U.S. should not take action to protect the environment	18%
U.S. should not take action to protect the environment	14%





SER	G2763	E2766	R2769	A2770	I2771	L2772	R2775	V2784	V2788	G2789	E2790	R2793	I2794	A2795	G2807	W2808	S2809	ALA	PHE	GLN																																			
D2572	L2573	E2574	T2575	L2576	L2577	K2578	V2579	R2585	H2593	F2594	F2595	L2596	E2597	S2598	Y2599	A2600	D2601	P2602	V2603	Q2604	W2605	T2608	Y2612	G2629	D2630	R2631	N2635	L2636	D2639	G2643	H2647	I2648	D2649	L2652	E2655	K2659	L2660	V2666	R2669	L2670	V2674	V2683	E2684	G2685											
V2686	F2687	E2702	L2706	S2707	V2708	L2709	E2710	V2711	L2712	R2713	V2714	L2717	F2718	S2719	W2720	L2721	L2722	S2723	P2724	L2725	R2726	R2727	M2728	K2729	L2730	Q2731	K2732	M2733	GLN	LEU	GLU	ASN	PHE	ASN	GLN	PRO	GLU	SER	GLY	ASN	ILE	THR	ASP	ALA	SER	ARG	ASP	PRO	LYS	ILE	GLN	ARG	ASN	ASN	VAL
A2362	V2363	K2364	K2365	L2366	L2367	D2368	L2369	L2370	K2371	S2372	N2373	S2377	L2383	F2387	F2388	N2389	Y2390	D2403	S2404	T2405	S2406	F2407	L2417	K2418	D2419	A2420	L2425	P2426	P2427	I2428	T2429	M2430	N2431	V2446	F2449	D2450	D2451	T2452	I2453	H2454	F2455	A2456	S2457	G2458	I2459	N2460	A2461	P2462	K2463	V2464	I2465				
S2250	A2251	H2253	Y2254	L2255	K2256	C2257	L2258	L2268	K2271	S2269	R2270	T2273	L2276	E2283	L2284	L2288	Q2289	K2290	Y2291	L2292	F2300	I2301	P2302	F2304	A2309	R2310	L2311	M2312	V2315	SER	K2317	F2318	Q2319	V2327	P2334	Y2335	L2341	V2345	L2354	D2355	A2356	G2357	S2358	R2359	Y2360	R2361									

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64713	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ANP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	F	0.67	0/64	0.74	0/86
2	A	0.20	1/16139 (0.0%)	0.43	10/22100 (0.0%)
2	B	0.15	0/16185	0.36	3/22124 (0.0%)
All	All	0.18	1/32388 (0.0%)	0.39	13/44310 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2658	LYS	CA-C	-12.38	1.36	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2334	PRO	CA-N-CD	-9.86	98.20	112.00
2	A	2661	PRO	N-CA-C	-6.93	103.89	113.53
2	B	2334	PRO	CA-N-CD	-6.40	103.04	112.00
2	B	2458	GLY	N-CA-C	-5.92	104.83	113.48
2	A	2457	SER	N-CA-C	5.72	117.84	108.52
2	A	2565	ILE	N-CA-C	-5.61	104.07	111.09
2	A	2564	LEU	N-CA-C	-5.51	105.28	111.28
2	A	2661	PRO	CA-C-N	-5.46	117.34	123.02
2	A	2661	PRO	C-N-CA	-5.46	117.34	123.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2334	PRO	N-CD-CG	-5.37	95.14	103.20
2	A	2563	LYS	CB-CA-C	5.22	120.83	110.17
2	A	650	ALA	N-CA-C	-5.09	105.91	111.82
2	B	2457	SER	N-CA-C	5.01	116.74	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	2657	GLY	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	64	0	59	6	0
2	A	15929	0	12395	416	0
2	B	15993	0	12577	381	0
3	A	31	0	13	3	0
3	B	31	0	13	4	0
All	All	32048	0	25057	799	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (799) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2195:LYS:HD3	2:A:2229:PHE:HB2	1.56	0.88
2:A:2018:LEU:HB3	2:A:2037:ARG:HH22	1.38	0.88
2:B:2459:ILE:HG22	2:B:2459:ILE:O	1.73	0.86
2:A:1399:LYS:HG3	2:A:1400:PRO:HD3	1.59	0.84
2:A:1492:MET:HE3	2:A:1492:MET:H	1.41	0.84
2:A:2560:THR:O	2:A:2564:LEU:HB2	1.78	0.83
2:B:2652:ILE:CG1	2:B:2726:ARG:HH12	1.92	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2334:PRO:HD2	2:B:2335:TYR:H	1.45	0.81
2:A:2457:SER:HA	2:A:2462:PRO:HG2	1.61	0.80
2:A:2460:ASN:CG	2:A:2482:GLY:HA3	2.05	0.80
2:A:1564:ASP:HB2	2:A:1579:ILE:HG13	1.64	0.80
2:A:2563:LYS:HA	2:A:2566:ALA:HB2	1.64	0.80
2:A:2563:LYS:HA	2:A:2566:ALA:CB	2.12	0.79
2:B:1366:LEU:HA	2:B:1369:ILE:HD12	1.63	0.79
2:B:2192:TYR:O	2:B:2196:LYS:N	2.15	0.79
2:A:2342:PHE:HA	2:A:2345:VAL:HG12	1.66	0.78
2:A:2521:VAL:HG12	2:A:2523:PRO:HD3	1.66	0.78
2:B:2660:LEU:HD23	2:B:2727:ARG:HB3	1.67	0.77
2:B:503:LEU:O	2:B:507:SER:N	2.19	0.76
2:A:1825:GLU:O	2:A:1830:ASN:ND2	2.18	0.76
2:A:2563:LYS:O	2:A:2566:ALA:HB3	1.84	0.76
2:B:1896:SER:HG	2:B:1898:GLU:N	1.83	0.75
2:B:2652:ILE:HG12	2:B:2726:ARG:HH12	1.49	0.75
2:A:1977:LEU:HA	2:A:1984:GLN:HB3	1.68	0.75
2:B:385:PHE:O	2:B:389:PHE:N	2.20	0.75
2:A:2562:ARG:HG3	2:A:2563:LYS:H	1.51	0.75
2:A:2162:ALA:HB2	2:A:2260:GLU:HB2	1.68	0.74
2:B:1547:PHE:HD2	2:B:1969:ALA:HB2	1.51	0.74
2:A:2499:VAL:HG11	2:A:2622:LEU:HD11	1.68	0.74
2:B:1346:ILE:HA	2:B:1349:ARG:HG3	1.70	0.74
2:A:2657:GLY:C	2:A:2659:LYS:N	2.45	0.73
2:B:2537:THR:HG22	2:B:2639:ASP:HA	1.70	0.73
1:F:69:GLN:CD	2:A:2662:VAL:HB	2.13	0.73
2:B:2659:LYS:HB3	2:B:2727:ARG:CZ	2.19	0.73
2:B:2460:ASN:C	2:B:2462:PRO:HD3	2.13	0.73
2:A:2126:LEU:HD23	2:A:2145:TYR:HE2	1.53	0.72
2:B:1580:ILE:HG23	2:B:1704:LEU:HD12	1.70	0.72
2:A:257:CYS:HA	2:A:260:ALA:HB3	1.71	0.72
2:A:1832:LEU:HD12	2:A:1848:LEU:HB3	1.71	0.72
2:B:1182:ILE:HD11	2:B:1212:ILE:HG13	1.71	0.72
2:B:2772:LEU:HA	2:B:2775:ARG:HD2	1.71	0.72
2:B:2354:LEU:HD12	2:B:2355:ASP:H	1.53	0.71
2:A:2685:GLY:H	2:A:2688:ARG:HG2	1.55	0.71
2:B:1925:LEU:HD12	2:B:1952:LYS:HE3	1.72	0.71
2:B:1553:ILE:HD11	2:B:1965:LEU:HD22	1.72	0.71
2:B:2044:LEU:HD21	2:B:2063:VAL:HB	1.72	0.71
2:B:2276:LEU:HD22	2:B:2310:ARG:HG2	1.72	0.71
2:B:1284:ASN:HB2	2:B:1430:ALA:HB1	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2657:GLY:O	2:A:2660:LEU:N	2.24	0.70
2:B:2486:LEU:HD23	2:B:2529:GLY:HA3	1.73	0.70
2:A:1367:VAL:O	2:A:1371:LEU:HD12	1.92	0.70
2:B:2301:ILE:HG13	2:B:2302:PRO:HD3	1.72	0.70
2:A:1478:ASN:HA	2:A:1481:PHE:HE1	1.56	0.70
2:B:1825:GLU:O	2:B:1830:ASN:ND2	2.27	0.68
2:A:2243:ARG:NH2	2:A:2244:SER:OG	2.25	0.68
2:B:1591:LEU:HD13	2:B:1693:PHE:HE1	1.58	0.68
2:A:1747:LEU:HD21	2:A:2601:ASP:HB2	1.76	0.68
2:A:2161:LYS:HG2	2:A:2165:TYR:CE1	2.27	0.68
2:B:2562:ARG:HG2	2:B:2807:GLY:HA2	1.76	0.68
2:B:2188:MET:HE2	2:B:2236:TYR:HB2	1.74	0.68
2:B:1375:ARG:HB2	2:B:1412:PHE:HE1	1.59	0.67
2:B:1588:ALA:HA	2:B:1591:LEU:HD12	1.76	0.67
2:B:2121:ILE:HA	2:B:2164:ILE:HD11	1.75	0.67
2:A:2018:LEU:HG	2:A:2037:ARG:HH12	1.59	0.67
2:A:2544:LEU:HA	2:A:2547:ALA:HB3	1.75	0.67
2:A:2420:ALA:HB3	2:A:2447:SER:HB2	1.77	0.67
2:A:2658:LYS:HD3	2:A:2664:GLU:HB2	1.77	0.67
2:B:1576:SER:O	2:B:1580:ILE:HG13	1.94	0.67
2:A:1576:SER:O	2:A:1580:ILE:HD12	1.95	0.67
2:B:1094:SER:H	2:B:1342:LEU:HD21	1.60	0.67
2:B:2652:ILE:CG1	2:B:2726:ARG:NH1	2.58	0.66
2:A:2665:CYS:SG	2:A:2803:LEU:HB3	2.35	0.66
2:B:2669:ARG:HH21	2:B:2809:SER:HA	1.60	0.66
2:A:2044:LEU:HD21	2:A:2063:VAL:HB	1.77	0.66
2:A:1688:THR:HA	2:A:1694:SER:HB3	1.78	0.66
2:B:1916:LEU:HD11	2:B:1952:LYS:HB2	1.78	0.66
2:A:2038:LYS:HD3	2:A:2071:TYR:HB2	1.78	0.65
2:A:2267:LEU:HD12	2:A:2267:LEU:H	1.61	0.65
2:B:1759:ASN:ND2	2:B:2550:VAL:O	2.29	0.65
2:B:2245:LYS:HE2	2:B:2249:GLN:HG3	1.79	0.65
2:B:2652:ILE:HG12	2:B:2726:ARG:NH1	2.12	0.65
2:A:1531:PHE:HE2	2:A:1535:LEU:HG	1.60	0.65
2:A:2672:ARG:HH21	2:A:2809:SER:HB3	1.60	0.64
2:B:2652:ILE:HG13	2:B:2726:ARG:HH12	1.62	0.64
2:A:2453:ILE:HG22	2:A:2455:PHE:HB3	1.79	0.64
2:B:1399:LYS:HG3	2:B:1400:PRO:HD3	1.78	0.64
2:B:1942:TYR:HE2	2:B:1979:ARG:HA	1.63	0.64
2:B:1930:LEU:HD21	2:B:2013:ILE:HG23	1.80	0.64
2:A:1654:THR:HA	2:A:1689:TYR:HA	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2489:ASP:O	2:B:2493:GLU:HG2	1.97	0.64
2:B:1748:TYR:O	2:B:1752:GLN:NE2	2.30	0.63
2:A:2106:LEU:HD23	2:A:2126:LEU:HD13	1.81	0.63
2:B:1334:LEU:HB2	2:B:1346:ILE:HG21	1.81	0.63
2:A:299:ALA:O	2:A:302:TYR:N	2.32	0.63
2:A:2192:TYR:O	2:A:2195:LYS:HG3	1.98	0.63
2:A:1377:LEU:HA	2:A:1380:ILE:HD12	1.80	0.63
2:B:1439:ASP:HA	2:B:1442:VAL:HG12	1.79	0.62
2:B:2284:LEU:O	2:B:2288:LEU:HG	1.99	0.62
2:A:2660:LEU:HD13	2:A:2661:PRO:HD2	1.80	0.62
2:A:2306:GLN:O	2:A:2310:ARG:HG2	1.98	0.62
2:B:157:CYS:O	2:B:161:ILE:N	2.33	0.62
2:A:1480:LEU:O	2:A:1485:HIS:ND1	2.31	0.62
2:B:1670:LEU:HB3	2:B:1709:PHE:HE2	1.64	0.62
2:A:2044:LEU:HD22	2:A:2060:ALA:HA	1.81	0.62
2:B:2635:ASN:HD22	2:B:2649:ASP:HB3	1.65	0.62
2:B:2013:ILE:O	2:B:2017:LEU:HB2	2.00	0.61
2:B:2766:GLU:OE1	2:B:2769:ARG:NH2	2.33	0.61
2:B:1975:LYS:O	2:B:1979:ARG:HG2	2.00	0.61
2:B:2390:TYR:HD2	2:B:2530:VAL:HG21	1.65	0.61
2:A:1949:ILE:HG21	2:A:1975:LYS:HD3	1.80	0.61
2:A:2071:TYR:CZ	2:A:2082:LYS:HB2	2.35	0.61
2:B:1742:CYS:HA	2:B:1745:ILE:HD12	1.80	0.61
2:A:1470:LYS:O	2:A:1474:ILE:HD12	2.00	0.61
2:A:1560:ILE:HG13	2:A:1561:PRO:HD2	1.81	0.61
2:A:2072:ARG:HH22	2:A:2082:LYS:HE2	1.66	0.61
2:A:2457:SER:OG	2:A:2462:PRO:HD2	2.01	0.61
2:B:2107:SER:HA	2:B:2126:LEU:HD11	1.81	0.61
2:A:1486:PHE:HA	2:A:1489:ARG:HB2	1.82	0.61
2:A:2044:LEU:HD12	2:A:2088:LEU:HD21	1.81	0.61
2:B:2040:TYR:O	2:B:2042:LEU:N	2.34	0.61
2:B:2465:ILE:HG22	2:B:2466:THR:H	1.65	0.61
2:B:1190:ALA:O	2:B:1194:THR:HG23	2.00	0.60
2:A:564:LYS:O	2:A:568:ILE:N	2.35	0.60
2:A:1988:ASP:O	2:A:1990:LEU:N	2.30	0.60
2:B:2790:GLU:O	2:B:2794:ILE:HG13	2.02	0.60
2:B:1718:GLN:O	2:B:1722:VAL:HG13	2.01	0.60
2:A:1874:GLY:HA3	2:A:2058:GLN:HB3	1.84	0.60
2:B:2341:LEU:O	2:B:2345:VAL:HG23	2.01	0.60
2:B:2725:LEU:H	2:B:2725:LEU:HD12	1.67	0.60
2:A:1942:TYR:O	2:A:1979:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1386:LEU:O	2:B:1390:ILE:HG13	2.03	0.59
2:B:1524:LYS:HE2	2:B:1960:GLU:HA	1.83	0.59
2:B:2334:PRO:HD2	2:B:2335:TYR:N	2.16	0.59
2:A:1286:VAL:O	2:A:1289:ASN:ND2	2.35	0.59
2:A:2402:VAL:CG1	2:A:2454:HIS:HA	2.33	0.59
2:B:1490:ILE:HB	2:B:1496:LEU:HD13	1.84	0.59
2:A:1495:TYR:O	2:A:1499:TYR:N	2.35	0.59
2:B:2359:ARG:O	2:B:2363:VAL:HG22	2.01	0.59
2:B:1323:ILE:O	2:B:1327:LEU:HG	2.02	0.59
2:A:2427:PRO:HG2	2:A:2430:MET:SD	2.43	0.59
2:A:2464:VAL:C	2:A:2465:ILE:HD12	2.28	0.59
2:B:2268:ILE:HD11	2:B:2300:PHE:HD1	1.68	0.59
2:A:2003:LEU:HD23	2:A:2004:HIS:H	1.67	0.58
2:B:1439:ASP:O	2:B:1441:TYR:N	2.36	0.58
2:B:2024:HIS:HB3	2:B:2027:LEU:HB2	1.84	0.58
3:B:2901:ANP:O1B	3:B:2901:ANP:O2G	2.21	0.58
2:A:2708:VAL:O	2:A:2712:LEU:HG	2.02	0.58
2:B:2273:THR:HB	2:B:2711:VAL:HG12	1.84	0.58
2:A:1492:MET:H	2:A:1492:MET:CE	2.14	0.58
2:A:2355:ASP:OD1	2:A:2359:ARG:NH2	2.37	0.58
2:A:2657:GLY:O	2:A:2658:LYS:C	2.45	0.58
2:A:1396:LYS:HD2	2:A:1437:TRP:HZ2	1.68	0.58
2:B:1384:GLN:O	2:B:1388:LEU:HD12	2.04	0.58
2:B:1390:ILE:HG23	2:B:1394:HIS:CE1	2.38	0.58
2:B:2110:LEU:HD22	2:B:2126:LEU:HD12	1.85	0.58
2:B:2165:TYR:O	2:B:2167:MET:N	2.36	0.58
2:A:1578:LEU:HD23	2:A:1579:ILE:HD13	1.85	0.58
2:B:2231:ILE:HD12	2:B:2234:ARG:HH21	1.69	0.58
2:A:2191:LEU:HA	2:A:2194:GLU:HG2	1.85	0.57
2:B:1631:ILE:HA	2:B:1635:ASP:HB2	1.85	0.57
2:B:2486:LEU:HD12	2:B:2489:ASP:HB2	1.85	0.57
2:B:2067:SER:HA	2:B:2070:LEU:HD12	1.84	0.57
2:B:2288:LEU:O	2:B:2292:LEU:HB2	2.04	0.57
2:B:2635:ASN:ND2	3:B:2901:ANP:O3G	2.37	0.57
2:B:1978:ILE:HG22	2:B:1979:ARG:HD2	1.87	0.57
2:A:2041:ILE:HA	2:A:2088:LEU:HD22	1.85	0.57
2:B:2496:PHE:O	2:B:2500:ASN:ND2	2.29	0.57
2:A:1178:ILE:HA	2:A:1181:LEU:HD12	1.87	0.57
2:A:2038:LYS:HB3	2:A:2081:LEU:HD21	1.87	0.57
2:B:2403:ASP:O	2:B:2455:PHE:N	2.34	0.57
2:A:2276:LEU:HD23	2:A:2318:PHE:HZ	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2288:LEU:HA	2:B:2291:TYR:HB2	1.87	0.57
2:B:2383:LEU:HG	2:B:2425:LEU:HD11	1.86	0.57
2:A:624:TYR:O	2:A:1941:ASN:ND2	2.38	0.57
2:A:1603:ILE:O	2:A:1607:ILE:HG22	2.05	0.57
2:A:1791:LEU:HB3	2:A:2680:ILE:HD13	1.87	0.57
2:A:1813:LEU:HD21	2:A:2606:PHE:CZ	2.39	0.56
2:B:2560:THR:HA	2:B:2563:LYS:HE3	1.87	0.56
2:A:2563:LYS:HD3	2:A:2566:ALA:CB	2.34	0.56
2:B:1365:TYR:CE2	2:B:1369:ILE:HD11	2.40	0.56
2:B:1697:ILE:HG23	2:B:1698:ILE:HD13	1.87	0.56
2:B:1925:LEU:HD21	2:B:1967:PHE:HB2	1.86	0.56
2:A:1395:LEU:HB3	2:A:1441:TYR:CZ	2.40	0.56
2:B:2702:GLU:O	2:B:2706:LEU:HB2	2.06	0.56
2:A:1478:ASN:HA	2:A:1481:PHE:CE1	2.39	0.56
2:A:2457:SER:OG	2:A:2462:PRO:CD	2.54	0.56
2:B:2719:SER:C	2:B:2721:LEU:H	2.13	0.56
2:B:2197:ASN:OD1	2:B:2201:GLN:NE2	2.39	0.56
2:B:1367:VAL:HG23	2:B:1394:HIS:HB3	1.88	0.56
2:B:1726:ILE:HD12	2:B:1767:VAL:HG11	1.87	0.56
2:B:2670:LEU:HB2	2:B:2795:ALA:HB1	1.87	0.56
2:B:2357:GLY:O	2:B:2361:ARG:NH2	2.38	0.56
2:B:2405:THR:OG1	2:B:2406:SER:N	2.39	0.56
2:B:2009:LEU:HD12	2:B:2013:ILE:HD11	1.88	0.55
2:A:1720:GLU:OE2	2:A:1720:GLU:N	2.38	0.55
2:A:1921:THR:HG22	2:A:1922:LYS:H	1.71	0.55
2:A:2407:PHE:HD2	2:A:2453:ILE:H	1.54	0.55
2:B:1820:TYR:HB2	2:B:2685:GLY:HA2	1.88	0.55
1:F:67:SER:HB2	2:A:2562:ARG:HH12	1.71	0.55
2:A:1471:ASN:O	2:A:1475:GLU:HG2	2.06	0.55
2:A:2453:ILE:C	2:A:2455:PHE:H	2.14	0.55
2:A:2429:THR:HG22	2:A:2522:ILE:HD13	1.88	0.55
2:A:1387:GLY:HA2	2:A:1390:ILE:HG12	1.87	0.55
2:A:114:PHE:HA	2:A:156:TYR:HA	1.89	0.55
2:A:1646:PHE:HD1	2:A:1648:TRP:H	1.54	0.55
2:A:1177:ILE:O	2:A:1181:LEU:HG	2.07	0.55
2:A:1772:SER:HB3	2:A:1794:HIS:CE1	2.42	0.55
2:A:1786:GLN:HB2	2:A:2602:PRO:HG3	1.87	0.55
2:A:2589:PRO:HD3	2:A:2672:ARG:HH12	1.72	0.55
2:A:1455:PHE:HB3	2:A:1476:VAL:HG13	1.88	0.55
2:A:1723:THR:HG21	2:A:1768:PRO:HG2	1.88	0.55
2:A:2223:SER:HA	2:A:2226:MET:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2698:LEU:HD12	2:A:2705:LEU:HD22	1.88	0.55
2:B:2724:PRO:HA	2:B:2727:ARG:CZ	2.37	0.55
2:B:1575:GLU:O	2:B:1579:ILE:HG12	2.06	0.55
2:B:2354:LEU:HG	2:B:2356:ALA:H	1.72	0.55
2:B:2710:GLU:HG3	2:B:2714:TYR:HE2	1.70	0.55
2:A:1879:ASN:O	2:A:1883:ILE:HG12	2.07	0.54
2:A:2106:LEU:HG	2:A:2126:LEU:HD22	1.88	0.54
2:B:1474:ILE:O	2:B:1478:ASN:ND2	2.38	0.54
2:B:2106:LEU:HG	2:B:2126:LEU:HG	1.89	0.54
2:A:2175:ASN:HB3	2:A:2246:MET:HE3	1.89	0.54
2:B:1547:PHE:CE1	2:B:1551:PRO:HB3	2.42	0.54
2:B:1928:GLU:OE1	2:B:1952:LYS:NZ	2.30	0.54
2:B:2367:LEU:HD13	2:B:2370:LEU:HD21	1.90	0.54
2:A:1470:LYS:HD3	2:A:1471:ASN:N	2.23	0.54
2:A:1528:ILE:HA	2:A:1531:PHE:HD1	1.71	0.54
2:A:1884:ASP:HA	2:A:1887:LYS:HD3	1.89	0.54
2:A:2503:LEU:O	2:A:2510:SER:OG	2.25	0.54
2:B:1455:PHE:H	2:B:1457:ARG:HH22	1.54	0.54
2:A:2587:TYR:O	2:A:2672:ARG:NH2	2.37	0.54
2:B:1919:LYS:HD3	2:B:1959:ASN:HD22	1.72	0.54
2:B:2708:VAL:O	2:B:2711:VAL:HG22	2.06	0.54
2:B:1284:ASN:HD22	2:B:1388:LEU:HD13	1.73	0.54
2:A:1264:THR:HG21	2:A:1287:SER:HA	1.89	0.54
2:B:2562:ARG:HH21	2:B:2809:SER:H	1.56	0.54
2:A:2003:LEU:HD23	2:A:2004:HIS:N	2.23	0.54
2:A:2334:PRO:O	2:A:2338:LEU:HB2	2.08	0.54
2:B:1177:ILE:O	2:B:1181:LEU:HD22	2.08	0.54
2:B:2366:ILE:O	2:B:2370:LEU:HD23	2.08	0.54
2:B:2724:PRO:HA	2:B:2727:ARG:NE	2.23	0.54
2:A:2352:GLU:H	2:A:2352:GLU:CD	2.16	0.54
2:B:2420:ALA:HA	2:B:2446:VAL:HG13	1.90	0.54
2:B:1904:TRP:HB3	2:B:1927:PHE:HD1	1.73	0.53
2:B:1701:ILE:HA	2:B:1704:LEU:HD23	1.91	0.53
2:B:1926:VAL:HG21	2:B:2009:LEU:HD11	1.89	0.53
2:A:1811:SER:HA	2:A:1819:TYR:HB2	1.90	0.53
2:A:2453:ILE:HG23	2:A:2464:VAL:O	2.09	0.53
2:B:1547:PHE:HE1	2:B:1551:PRO:HB3	1.74	0.53
2:B:2360:TYR:CE2	2:B:2364:LYS:HD2	2.43	0.53
2:B:2464:VAL:HG11	2:B:2476:LYS:HE3	1.90	0.53
2:B:1339:ASP:O	2:B:1343:GLN:HG2	2.08	0.53
2:A:1442:VAL:HG12	2:A:1456:LEU:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1596:ASP:O	2:A:1600:ASP:HB2	2.09	0.53
2:B:2652:ILE:HD12	2:B:2730:LYS:HG2	1.90	0.53
2:A:2334:PRO:HA	2:A:2338:LEU:HD23	1.91	0.52
2:B:1388:LEU:HB3	2:B:1434:PHE:CE2	2.44	0.52
2:A:2486:LEU:HB3	2:A:2523:PRO:HB3	1.91	0.52
2:B:1993:LEU:O	2:B:1997:LYS:N	2.33	0.52
2:A:2272:CYS:O	2:A:2276:LEU:HD12	2.09	0.52
2:B:2018:LEU:O	2:B:2020:LEU:N	2.42	0.52
2:A:1323:ILE:HG21	2:A:1361:ILE:HD12	1.92	0.52
2:A:2563:LYS:C	2:A:2566:ALA:HB3	2.34	0.52
2:B:1942:TYR:CE2	2:B:1979:ARG:HA	2.43	0.52
1:F:69:GLN:OE1	2:A:2662:VAL:HB	2.08	0.52
2:A:1942:TYR:HB2	2:A:1979:ARG:HH21	1.75	0.52
2:A:2568:LYS:HG3	2:A:2576:ARG:HG2	1.91	0.52
2:B:1093:ARG:H	2:B:1342:LEU:HD11	1.74	0.52
2:B:1691:VAL:O	2:B:1693:PHE:N	2.43	0.52
2:B:1703:HIS:ND1	2:B:1748:TYR:HD2	2.08	0.52
2:A:2562:ARG:HG3	2:A:2563:LYS:N	2.22	0.52
2:B:2631:ARG:HD2	2:B:2647:HIS:CE1	2.45	0.52
2:B:2669:ARG:HG3	2:B:2808:TRP:CZ3	2.45	0.52
2:A:2480:LYS:NZ	3:A:2901:ANP:H8	2.25	0.52
2:A:2563:LYS:CA	2:A:2566:ALA:HB3	2.40	0.52
2:B:1666:GLU:OE2	2:B:1725:LEU:HB2	2.10	0.52
2:B:2312:MET:N	2:B:2319:GLN:OE1	2.42	0.52
2:A:2185:PHE:HE2	2:A:2243:ARG:HD3	1.74	0.51
2:B:2666:VAL:HG23	2:B:2795:ALA:HA	1.93	0.51
2:B:2526:LEU:H	2:B:2526:LEU:HD12	1.75	0.51
2:B:2702:GLU:HG3	2:B:2706:LEU:HD23	1.92	0.51
2:A:1543:MET:HE3	2:A:1543:MET:HA	1.93	0.51
2:A:2346:SER:OG	2:A:2347:ASN:ND2	2.43	0.51
2:B:1577:LYS:HA	2:B:1580:ILE:HD12	1.92	0.51
2:B:2460:ASN:O	2:B:2462:PRO:HD3	2.10	0.51
2:B:2670:LEU:HD13	2:B:2683:VAL:HG11	1.92	0.51
2:B:1432:GLN:HA	2:B:1435:TYR:CD2	2.45	0.51
2:B:2599:TYR:CD2	2:B:2608:THR:HG21	2.45	0.51
2:B:2669:ARG:HG3	2:B:2808:TRP:CH2	2.45	0.51
2:B:2496:PHE:HA	2:B:2499:VAL:HG22	1.91	0.51
2:B:2387:PHE:HE1	2:B:2428:ILE:HG21	1.75	0.51
2:A:2537:THR:HG22	2:A:2639:ASP:HA	1.91	0.51
2:B:1691:VAL:O	2:B:1694:SER:N	2.43	0.51
2:B:1697:ILE:O	2:B:1701:ILE:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2459:ILE:HG22	2:A:2460:ASN:HD22	1.76	0.51
2:A:2713:ARG:NE	2:A:2771:ILE:HG21	2.25	0.51
3:A:2901:ANP:O2G	3:A:2901:ANP:O1B	2.29	0.51
2:B:2218:LEU:O	2:B:2222:HIS:N	2.41	0.51
2:B:2359:ARG:HH12	2:B:2717:LEU:HD21	1.76	0.51
2:A:1813:LEU:HD21	2:A:2606:PHE:HZ	1.75	0.50
2:A:2512:ARG:HH21	2:A:2693:PHE:HE2	1.59	0.50
2:B:1682:SER:O	2:B:1687:SER:N	2.43	0.50
2:A:1386:LEU:O	2:A:1390:ILE:HG23	2.12	0.50
2:A:2188:MET:HE1	2:A:2236:TYR:HA	1.93	0.50
2:A:2453:ILE:C	2:A:2455:PHE:N	2.65	0.50
2:A:2625:VAL:O	2:A:2774:VAL:HG22	2.11	0.50
2:B:2123:TYR:HD1	2:B:2145:TYR:HA	1.75	0.50
2:B:2198:ASP:N	2:B:2198:ASP:OD1	2.43	0.50
2:B:1977:LEU:HG	2:B:1984:GLN:HB3	1.92	0.50
2:A:1726:ILE:HG21	2:A:1746:LEU:HD21	1.94	0.50
2:B:1520:TRP:HB3	2:B:1543:MET:SD	2.52	0.50
2:A:2360:TYR:HA	2:A:2363:VAL:HG12	1.94	0.50
2:A:2770:ALA:O	2:A:2774:VAL:HG23	2.12	0.50
2:A:1605:ASP:HB2	2:A:1645:SER:OG	2.12	0.50
2:A:2157:ASN:HA	2:A:2161:LYS:HD2	1.92	0.50
2:A:2236:TYR:HD2	2:A:2237:LEU:HD23	1.77	0.50
2:B:1178:ILE:O	2:B:1182:ILE:HG23	2.11	0.50
2:A:2188:MET:O	2:A:2191:LEU:HD12	2.11	0.50
2:B:1334:LEU:HA	2:B:1346:ILE:HD13	1.92	0.50
2:B:2639:ASP:O	2:B:2643:GLY:N	2.40	0.50
2:A:2496:PHE:HB3	2:A:2518:THR:HG22	1.93	0.50
2:B:1502:GLN:HA	2:B:1535:LEU:HD11	1.92	0.50
2:B:1904:TRP:HD1	2:B:1927:PHE:HB2	1.77	0.50
2:B:2301:ILE:HA	2:B:2304:PHE:HB2	1.94	0.50
2:B:2601:ASP:HB2	2:B:2602:PRO:HD2	1.94	0.50
2:A:1941:ASN:OD1	2:A:1944:HIS:N	2.43	0.50
2:A:2150:LEU:HA	2:A:2153:MET:HG2	1.94	0.50
2:A:2336:HIS:NE2	2:A:2432:VAL:HG23	2.27	0.50
2:A:2544:LEU:O	2:A:2548:HIS:HB2	2.12	0.50
2:A:2397:ASN:ND2	2:A:2461:ALA:HB2	2.27	0.49
2:B:1627:LYS:HZ3	2:B:1630:ILE:HD11	1.77	0.49
2:B:2001:SER:HA	2:B:2511:GLN:HA	1.93	0.49
2:A:1580:ILE:HG23	2:A:1704:LEU:HB3	1.94	0.49
2:A:2013:ILE:HA	2:A:2016:VAL:HG12	1.94	0.49
2:A:1909:TRP:CZ3	2:A:1930:LEU:HB3	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1946:GLU:HG3	2:A:1975:LYS:HZ1	1.78	0.49
2:B:2165:TYR:CD2	2:B:2256:LYS:HB3	2.48	0.49
1:F:69:GLN:NE2	2:A:2662:VAL:HB	2.27	0.49
2:A:2226:MET:SD	2:A:2227:SER:N	2.85	0.49
2:A:2309:ALA:HA	2:A:2359:ARG:HD3	1.94	0.49
2:A:2330:GLY:O	2:A:2334:PRO:HD3	2.11	0.49
2:A:2594:PHE:HE2	2:A:2638:ILE:HG21	1.76	0.49
2:B:1967:PHE:CD1	2:B:1967:PHE:C	2.91	0.49
2:B:2521:VAL:HG12	2:B:2523:PRO:HD3	1.93	0.49
2:A:1595:TYR:CD1	2:A:1599:LEU:HD11	2.46	0.49
2:A:2565:ILE:HD12	2:A:2568:LYS:HD3	1.95	0.49
2:B:2459:ILE:O	2:B:2459:ILE:CG2	2.46	0.49
2:A:943:TYR:O	2:A:947:ARG:CB	2.61	0.49
2:A:1893:ASP:O	2:A:1895:CYS:N	2.41	0.49
2:A:2153:MET:HE2	2:A:2161:LYS:HG3	1.93	0.49
2:A:2713:ARG:HH21	2:A:2771:ILE:HD13	1.76	0.49
2:B:1446:LEU:HD22	2:B:1457:ARG:HD2	1.93	0.49
2:B:1835:ALA:HB3	2:B:1845:ILE:HD13	1.95	0.49
2:A:1759:ASN:HD21	2:A:2551:TYR:HA	1.78	0.49
2:A:2402:VAL:HG11	2:A:2407:PHE:CD2	2.48	0.49
2:B:2202:LEU:HD22	2:B:2222:HIS:CE1	2.48	0.49
2:B:2707:SER:O	2:B:2711:VAL:HG13	2.13	0.49
2:A:2563:LYS:HD3	2:A:2566:ALA:HB1	1.94	0.49
2:B:1332:ILE:HG23	2:B:1650:LYS:HE2	1.94	0.49
2:B:1363:SER:O	2:B:1367:VAL:HG12	2.12	0.49
2:A:2512:ARG:O	2:A:2614:ARG:NH1	2.46	0.49
2:B:2629:GLY:HA3	2:B:2652:ILE:HG22	1.94	0.48
2:A:2459:ILE:HG22	2:A:2460:ASN:ND2	2.28	0.48
2:A:2565:ILE:HA	2:A:2568:LYS:HB3	1.94	0.48
2:A:2624:HIS:ND1	2:A:2791:LEU:HD11	2.28	0.48
2:A:2639:ASP:O	2:A:2640:LYS:HB2	2.14	0.48
2:B:574:LEU:HA	2:B:578:GLN:N	2.28	0.48
2:A:1321:SER:O	2:A:1325:LEU:HG	2.14	0.48
2:A:1524:LYS:NZ	2:A:1960:GLU:HA	2.27	0.48
2:A:1810:LEU:HB3	2:A:1819:TYR:HA	1.95	0.48
2:A:2767:ALA:O	2:A:2771:ILE:HG22	2.12	0.48
2:B:1353:PHE:O	2:B:1357:SER:N	2.46	0.48
2:A:1875:PHE:HB3	2:A:1878:LEU:HD12	1.96	0.48
2:A:1933:VAL:HG21	2:A:1974:LEU:HD11	1.94	0.48
2:A:2057:LEU:HD21	2:A:2096:ARG:HG2	1.96	0.48
2:B:1512:LEU:HD13	2:B:1542:ILE:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2719:SER:C	2:B:2721:LEU:N	2.69	0.48
2:A:1747:LEU:HD12	2:A:1750:ARG:HD3	1.96	0.48
2:A:1827:SER:OG	2:A:1828:PHE:N	2.47	0.48
2:B:1600:ASP:HA	2:B:1603:ILE:HD12	1.96	0.48
2:B:1747:LEU:HD21	2:B:2602:PRO:HD3	1.94	0.48
1:F:71:LEU:HA	2:A:2660:LEU:HD11	1.96	0.48
2:A:2402:VAL:HG13	2:A:2454:HIS:CD2	2.48	0.48
2:B:2771:ILE:O	2:B:2775:ARG:HG3	2.14	0.48
2:A:1469:THR:OG1	2:A:1472:GLU:HG2	2.14	0.48
2:A:1574:GLU:HA	2:A:1577:LYS:HE2	1.95	0.48
2:A:2256:LYS:HD3	2:A:2291:TYR:HE2	1.79	0.48
2:B:1367:VAL:O	2:B:1371:LEU:HG	2.13	0.48
2:A:1518:GLU:OE1	2:A:1521:LYS:HB3	2.14	0.48
2:A:2568:LYS:HB2	2:A:2579:VAL:HG21	1.96	0.48
2:B:2044:LEU:HD22	2:B:2060:ALA:HA	1.96	0.48
2:B:2732:LYS:HB3	2:B:2732:LYS:HE3	1.57	0.48
2:A:1829:LYS:O	2:A:1833:LEU:HG	2.14	0.48
2:A:2354:LEU:HG	2:A:2356:ALA:H	1.79	0.48
2:A:2654:PHE:CD2	2:A:2720:TRP:HD1	2.32	0.48
2:B:1438:PHE:O	2:B:1442:VAL:N	2.32	0.48
2:B:1523:TYR:CD2	2:B:1524:LYS:HG2	2.49	0.48
2:B:2368:ASP:O	2:B:2372:VAL:HG23	2.13	0.48
2:A:2402:VAL:HG12	2:A:2454:HIS:HA	1.94	0.47
2:A:2558:LEU:O	2:A:2562:ARG:HG2	2.13	0.47
2:A:2336:HIS:NE2	2:A:2432:VAL:O	2.46	0.47
2:A:2480:LYS:HZ1	3:A:2901:ANP:H8	1.79	0.47
2:A:2684:GLU:HG3	2:A:2688:ARG:HH11	1.79	0.47
2:B:1364:ASN:OD1	2:B:1365:TYR:N	2.47	0.47
2:B:2153:MET:HE3	2:B:2165:TYR:CZ	2.49	0.47
2:B:2235:GLU:O	2:B:2239:MET:HG2	2.14	0.47
2:B:2407:PHE:CZ	2:B:2451:ASP:HA	2.48	0.47
2:A:2301:ILE:HG12	2:A:2302:PRO:HD3	1.96	0.47
2:A:2310:ARG:HB2	2:A:2322:LEU:HD21	1.96	0.47
2:A:2520:LYS:HG2	2:A:2522:ILE:HD11	1.97	0.47
2:A:2126:LEU:HD12	2:A:2126:LEU:HA	1.73	0.47
2:A:1327:LEU:HD11	2:A:1369:ILE:HG23	1.96	0.47
2:A:1347:SER:O	2:A:1350:LEU:HD12	2.15	0.47
2:A:1350:LEU:HA	2:A:1353:PHE:CD2	2.49	0.47
2:A:1390:ILE:O	2:A:1394:HIS:ND1	2.48	0.47
2:A:1882:TYR:CZ	2:A:1886:LEU:HD11	2.49	0.47
2:B:801:LEU:HA	2:B:805:THR:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2575:THR:O	2:B:2578:LYS:HG3	2.13	0.47
2:A:1818:ALA:C	2:A:1820:TYR:H	2.23	0.47
2:A:2265:ASP:O	2:A:2268:ILE:HG22	2.14	0.47
2:A:2349:PRO:HB2	2:A:2352:GLU:OE2	2.14	0.47
2:A:2536:ASP:N	2:A:2536:ASP:OD1	2.48	0.47
2:B:1283:ALA:HB3	2:B:1389:GLY:HA2	1.95	0.47
2:A:1316:PHE:HA	2:A:1319:ILE:HD11	1.97	0.47
2:A:1548:PHE:HB3	2:A:1549:LYS:HD3	1.95	0.47
2:A:2161:LYS:HG2	2:A:2165:TYR:HE1	1.76	0.47
2:A:2227:SER:O	2:A:2230:ILE:HG22	2.15	0.47
2:A:2431:ASN:HA	2:A:2520:LYS:HE3	1.96	0.47
2:A:2657:GLY:O	2:A:2659:LYS:N	2.48	0.47
2:B:1122:ILE:O	2:B:1124:SER:N	2.47	0.47
2:B:1985:PHE:CD1	2:B:1985:PHE:C	2.93	0.47
2:B:2165:TYR:CZ	2:B:2256:LYS:HD3	2.49	0.47
2:B:2309:ALA:HA	2:B:2359:ARG:NH2	2.30	0.47
2:A:1913:PRO:HB2	2:A:1928:GLU:HG2	1.95	0.47
2:A:2264:ASN:HB3	2:A:2267:LEU:HD11	1.96	0.47
2:A:2670:LEU:HD12	2:A:2670:LEU:HA	1.76	0.47
2:B:1664:LYS:HA	2:B:1698:ILE:HG21	1.97	0.47
2:A:1255:LEU:HA	2:A:1349:ARG:NH2	2.30	0.47
2:A:2453:ILE:O	2:A:2455:PHE:N	2.43	0.47
2:A:2659:LYS:HE2	2:A:2659:LYS:HB2	1.61	0.47
2:B:2086:ASP:O	2:B:2090:SER:OG	2.30	0.47
2:B:2355:ASP:O	2:B:2359:ARG:HG3	2.15	0.47
2:B:2468:LEU:HA	2:B:2474:THR:HB	1.97	0.47
2:B:2670:LEU:HD11	2:B:2687:PHE:CZ	2.50	0.47
2:A:1884:ASP:OD1	2:A:1884:ASP:N	2.47	0.46
2:A:2535:GLN:O	2:A:2537:THR:HG23	2.15	0.46
2:A:2595:PHE:CE2	2:A:2609:GLN:HA	2.50	0.46
2:B:1093:ARG:H	2:B:1342:LEU:CD1	2.28	0.46
2:B:1500:PHE:HD1	2:B:1500:PHE:H	1.63	0.46
2:B:2137:LYS:HG2	2:B:2139:GLU:H	1.79	0.46
2:B:1657:ASP:OD2	2:B:1688:THR:OG1	2.33	0.46
2:B:2016:VAL:O	2:B:2020:LEU:HG	2.14	0.46
2:A:1952:LYS:HA	2:A:1952:LYS:HD3	1.72	0.46
2:A:2094:TRP:CZ3	2:A:2099:LYS:HB3	2.50	0.46
2:A:2306:GLN:HE21	2:A:2712:LEU:HD23	1.80	0.46
2:A:2636:ILE:C	2:A:2637:LEU:HD23	2.41	0.46
2:B:1278:GLN:O	2:B:1282:PHE:N	2.49	0.46
2:B:2568:LYS:HD2	2:B:2579:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2655:GLU:OE1	2:B:2659:LYS:NZ	2.42	0.46
2:A:351:ARG:H	2:A:367:PRO:N	2.14	0.46
2:A:1759:ASN:HB3	2:A:1762:GLU:H	1.81	0.46
2:A:2226:MET:HA	2:A:2229:PHE:CE2	2.50	0.46
2:B:2169:ALA:HA	2:B:2250:SER:HA	1.97	0.46
2:B:2407:PHE:HE1	2:B:2417:LEU:HD11	1.81	0.46
2:A:594:TYR:C	2:A:596:LEU:H	2.22	0.46
2:A:2087:PHE:HA	2:A:2106:LEU:HD13	1.98	0.46
2:A:2160:GLU:O	2:A:2164:ILE:HG12	2.16	0.46
2:B:1371:LEU:HB3	2:B:1412:PHE:CE2	2.50	0.46
2:B:2045:LEU:O	2:B:2049:GLU:N	2.24	0.46
2:A:1925:LEU:HD11	2:A:1952:LYS:HD2	1.96	0.46
2:A:2118:PHE:N	2:A:2119:PRO:HD3	2.31	0.46
2:A:2710:GLU:HA	2:A:2713:ARG:HG3	1.97	0.46
2:B:1020:ASP:O	2:B:1024:LEU:N	2.38	0.46
2:B:2309:ALA:HB2	2:B:2717:LEU:HD11	1.98	0.46
2:A:1382:CYS:SG	2:A:1383:THR:N	2.89	0.46
2:A:1687:SER:HA	2:A:1693:PHE:CG	2.51	0.46
2:B:1390:ILE:O	2:B:1394:HIS:ND1	2.38	0.46
2:B:1722:VAL:HA	2:B:1725:LEU:HG	1.98	0.46
2:A:2429:THR:HG21	2:A:2477:GLN:HG3	1.96	0.46
2:B:1375:ARG:HB2	2:B:1412:PHE:CE1	2.46	0.46
2:B:2669:ARG:NH2	2:B:2809:SER:HA	2.28	0.46
2:B:1580:ILE:HD13	2:B:1708:GLU:HG2	1.96	0.46
2:B:1599:LEU:O	2:B:1603:ILE:HG13	2.16	0.45
2:B:2593:HIS:HA	2:B:2596:LEU:HG	1.97	0.45
2:A:1652:GLN:HB3	2:A:1689:TYR:CD1	2.51	0.45
2:A:1687:SER:O	2:A:1693:PHE:HB3	2.16	0.45
2:A:2259:SER:HB2	2:A:2295:LEU:HD22	1.99	0.45
2:B:2011:LEU:HD11	2:B:2053:ILE:HD12	1.98	0.45
2:A:1687:SER:HA	2:A:1693:PHE:CD2	2.51	0.45
2:A:2325:ILE:O	2:A:2329:VAL:HG22	2.16	0.45
2:B:2010:LEU:HB2	2:B:2053:ILE:HG21	1.99	0.45
2:A:1602:PHE:CD1	2:A:1686:LEU:HD21	2.52	0.45
2:A:1682:SER:O	2:A:1685:LEU:HG	2.17	0.45
2:A:1720:GLU:O	2:A:1723:THR:HG22	2.17	0.45
2:A:2311:LEU:HA	2:A:2322:LEU:HD23	1.98	0.45
2:A:1762:GLU:O	2:A:1766:TRP:N	2.50	0.45
2:B:2449:PHE:HD1	2:B:2465:ILE:HG21	1.81	0.45
2:B:2461:ALA:O	2:B:2463:LYS:NZ	2.50	0.45
2:A:2282:ASP:HB2	2:A:2317:LYS:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2471:ASN:OD1	2:A:2471:ASN:N	2.50	0.45
2:B:2066:LEU:O	2:B:2070:LEU:HG	2.15	0.45
2:B:2459:ILE:HG21	2:B:2733:MET:SD	2.57	0.45
2:A:1363:SER:HB3	2:A:1366:LEU:HD23	1.98	0.45
2:A:1410:ALA:HB1	2:A:1486:PHE:HZ	1.81	0.45
2:A:1750:ARG:NH2	2:A:2597:GLU:H	2.15	0.45
2:A:2153:MET:HE3	2:A:2153:MET:HA	1.99	0.45
2:A:2480:LYS:NZ	2:A:2531:ILE:HD11	2.32	0.45
2:B:1625:PHE:HB2	2:B:1626:PRO:HD3	1.99	0.45
2:B:2453:ILE:HG22	2:B:2465:ILE:HG13	1.99	0.45
2:A:1212:ILE:HA	2:A:1215:TYR:CE2	2.51	0.45
2:A:2037:ARG:HA	2:A:2037:ARG:NH1	2.32	0.45
2:A:2559:SER:HA	2:A:2562:ARG:HG2	1.98	0.45
2:B:1341:GLU:O	2:B:1345:THR:HG23	2.16	0.45
2:B:1580:ILE:HG13	2:B:1580:ILE:H	1.64	0.45
2:A:1351:CYS:HA	2:A:1354:LEU:HD12	1.98	0.45
2:B:1043:ASP:O	2:B:1047:PHE:N	2.50	0.45
2:B:2130:LEU:HD22	2:B:2135:SER:HB3	1.99	0.45
2:B:2389:ASN:ND2	2:B:2419:ASP:OD2	2.49	0.45
2:A:2239:MET:HE2	2:A:2239:MET:HA	1.98	0.45
2:A:1563:THR:HG23	2:A:1565:PRO:HD2	1.99	0.44
2:A:1722:VAL:O	2:A:1725:LEU:HG	2.17	0.44
2:B:2188:MET:O	2:B:2188:MET:HE3	2.17	0.44
2:B:2327:TYR:N	2:B:2366:ILE:HD11	2.32	0.44
2:B:2556:TRP:HB3	2:B:2560:THR:HB	1.99	0.44
2:B:2729:LYS:HD3	2:B:2729:LYS:HA	1.73	0.44
2:A:1366:LEU:O	2:A:1369:ILE:HG22	2.17	0.44
2:A:1464:ARG:O	2:A:1464:ARG:HG3	2.17	0.44
2:A:2327:TYR:CZ	2:A:2369:LEU:HG	2.52	0.44
2:B:1065:SER:C	2:B:1103:LEU:HA	2.43	0.44
2:A:1894:GLU:HA	2:A:1899:VAL:HG21	1.98	0.44
2:A:2563:LYS:HA	2:A:2566:ALA:HB3	1.91	0.44
2:A:2627:GLY:HA3	2:A:2655:GLU:H	1.81	0.44
2:B:2231:ILE:HG23	2:B:2234:ARG:NH2	2.32	0.44
2:A:1941:ASN:CG	2:A:1943:LEU:H	2.25	0.44
2:A:2188:MET:CE	2:A:2236:TYR:HA	2.47	0.44
2:B:1444:ALA:HA	2:B:1447:ASN:ND2	2.33	0.44
2:B:1670:LEU:HD21	2:B:1722:VAL:HG12	1.99	0.44
2:B:2178:SER:O	2:B:2182:THR:HG22	2.17	0.44
2:A:1501:TRP:O	2:A:1505:ASP:N	2.46	0.44
2:A:1562:LYS:O	2:A:1562:LYS:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1909:TRP:CH2	2:A:1930:LEU:HB3	2.52	0.44
2:A:2545:ASP:O	2:A:2549:LYS:HG2	2.17	0.44
2:A:2595:PHE:HE2	2:A:2609:GLN:HA	1.81	0.44
2:B:2521:VAL:C	2:B:2522:ILE:HD12	2.42	0.44
2:B:2572:ASP:OD2	2:B:2574:GLU:N	2.51	0.44
2:B:2596:LEU:C	2:B:2598:SER:H	2.25	0.44
2:A:2231:ILE:O	2:A:2234:ARG:HG2	2.17	0.44
2:B:1527:ASP:C	2:B:1528:ILE:HD13	2.42	0.44
2:B:1772:SER:HB2	2:B:1794:HIS:CE1	2.53	0.44
2:A:1392:ARG:O	2:A:1396:LYS:HG3	2.18	0.44
2:A:1548:PHE:HE1	2:A:1969:ALA:HB1	1.82	0.44
2:A:2543:TYR:CE2	2:A:2594:PHE:HB2	2.53	0.44
2:B:1390:ILE:HG13	2:B:1390:ILE:H	1.68	0.44
2:B:1548:PHE:CZ	2:B:1973:ASP:HB2	2.52	0.44
2:B:2226:MET:O	2:B:2230:ILE:HG12	2.18	0.44
2:B:2535:GLN:O	2:B:2537:THR:HG23	2.17	0.44
2:B:2543:TYR:CZ	2:B:2594:PHE:HD2	2.36	0.44
2:A:1852:ASN:ND2	2:A:1857:ASN:HB2	2.33	0.44
2:A:2629:GLY:N	2:A:2652:ILE:O	2.49	0.44
2:B:1688:THR:OG1	2:B:1688:THR:O	2.35	0.44
2:B:1750:ARG:HB3	2:B:2597:GLU:OE1	2.18	0.44
2:B:1366:LEU:O	2:B:1370:VAL:HG23	2.17	0.44
2:B:1681:HIS:O	2:B:1685:LEU:HG	2.18	0.44
2:A:1975:LYS:O	2:A:1979:ARG:HG2	2.18	0.43
2:B:1284:ASN:CB	2:B:1430:ALA:HB1	2.43	0.43
2:B:1929:VAL:O	2:B:1933:VAL:HG13	2.17	0.43
2:B:2129:TRP:O	2:B:2132:THR:OG1	2.33	0.43
2:A:1547:PHE:HD2	2:A:1969:ALA:HB2	1.83	0.43
2:A:2487:ARG:HD3	2:A:2717:LEU:HD13	2.00	0.43
2:A:2803:LEU:HD23	2:A:2803:LEU:O	2.18	0.43
2:B:1388:LEU:HB3	2:B:1434:PHE:HE2	1.82	0.43
2:B:2652:ILE:HG13	2:B:2726:ARG:NH1	2.28	0.43
2:A:1580:ILE:O	2:A:1584:ILE:HG12	2.17	0.43
2:A:1587:LYS:HD3	2:A:1701:ILE:HG23	1.99	0.43
2:B:1719:LYS:O	2:B:1722:VAL:HG22	2.18	0.43
2:B:2007:PHE:HB2	2:B:2053:ILE:HG23	2.00	0.43
2:B:2427:PRO:HD2	2:B:2430:MET:SD	2.58	0.43
2:B:2522:ILE:HD12	2:B:2522:ILE:N	2.33	0.43
2:A:1273:PHE:HA	2:A:1276:TYR:CD2	2.54	0.43
2:A:1427:LYS:O	2:A:1431:ILE:HG12	2.19	0.43
2:B:1460:ILE:HD12	2:B:1460:ILE:HA	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2493:GLU:OE1	2:B:2518:THR:OG1	2.31	0.43
2:A:1946:GLU:OE2	2:A:1979:ARG:NH1	2.52	0.43
2:A:2356:ALA:O	2:A:2359:ARG:HG2	2.17	0.43
2:B:2568:LYS:HB3	2:B:2568:LYS:HE2	1.75	0.43
3:B:2901:ANP:O2G	3:B:2901:ANP:O1A	2.36	0.43
2:A:1946:GLU:HG3	2:A:1979:ARG:HH12	1.83	0.43
2:A:1951:LYS:HE3	2:A:1951:LYS:HB2	1.72	0.43
2:A:2103:ILE:HD12	2:A:2130:LEU:HD23	1.99	0.43
2:A:2458:GLY:H	2:A:2462:PRO:HG2	1.83	0.43
2:A:2343:SER:HB2	2:A:2523:PRO:O	2.18	0.43
2:A:2393:LEU:HD11	2:A:2465:ILE:HD11	2.01	0.43
2:B:2428:ILE:HB	2:B:2522:ILE:HG21	2.01	0.43
2:A:1205:TYR:CZ	2:A:1212:ILE:HG13	2.54	0.43
2:A:1435:TYR:HB3	2:A:1464:ARG:HD3	2.00	0.43
2:A:2298:LYS:NZ	2:A:2436:ASP:OD1	2.32	0.43
2:A:2332:ASN:ND2	2:A:2438:GLY:HA3	2.34	0.43
2:B:1650:LYS:HA	2:B:1650:LYS:HD2	1.63	0.43
2:B:1741:THR:O	2:B:1745:ILE:HG13	2.18	0.43
2:B:1758:LEU:N	2:B:1762:GLU:OE2	2.51	0.43
2:B:1777:THR:O	2:B:1781:CYS:N	2.51	0.43
2:B:1790:PHE:O	2:B:1793:ILE:HG22	2.18	0.43
2:B:2429:THR:HA	2:B:2522:ILE:HD13	1.99	0.43
2:B:2585:ARG:HA	2:B:2585:ARG:NE	2.34	0.43
2:A:1643:GLU:OE1	2:A:1645:SER:HB2	2.19	0.43
2:A:1935:ASN:ND2	2:A:1935:ASN:C	2.76	0.43
2:A:2165:TYR:HB3	2:A:2253:HIS:ND1	2.34	0.43
2:A:2251:ILE:HG21	2:A:2288:LEU:HD13	2.00	0.43
2:A:2624:HIS:CE1	2:A:2791:LEU:HD11	2.54	0.43
2:A:2720:TRP:CG	2:A:2767:ALA:HB2	2.54	0.43
2:B:651:TRP:O	2:B:655:THR:N	2.52	0.43
2:B:1448:PHE:C	2:B:1448:PHE:CD1	2.97	0.43
2:B:2199:ILE:O	2:B:2203:GLU:HG2	2.19	0.43
2:B:2520:LYS:NZ	2:B:2522:ILE:HD11	2.33	0.43
2:A:1496:LEU:HG	2:A:1527:ASP:O	2.18	0.43
2:B:1658:SER:HA	2:B:1691:VAL:HG23	2.01	0.43
2:B:2174:ASN:O	2:B:2178:SER:N	2.52	0.43
2:A:626:PRO:N	2:A:1943:LEU:HB3	2.34	0.42
2:A:1070:LYS:O	2:A:1074:LYS:N	2.51	0.42
2:A:2698:LEU:CD1	2:A:2705:LEU:HD22	2.50	0.42
2:A:2713:ARG:NH2	2:A:2771:ILE:HD13	2.34	0.42
2:B:788:ASP:O	2:B:791:LYS:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2491:VAL:O	2:B:2495:VAL:HG23	2.19	0.42
2:A:1523:TYR:CE1	2:A:1524:LYS:HE2	2.54	0.42
2:B:1785:GLU:OE1	2:B:1785:GLU:N	2.40	0.42
2:B:2076:LEU:HG	2:B:2077:ALA:N	2.35	0.42
2:B:2114:ASN:HB2	2:B:2117:ILE:HB	2.00	0.42
2:B:2178:SER:HB3	2:B:2181:LEU:HB2	2.01	0.42
2:B:2405:THR:HG23	2:B:2453:ILE:HG13	2.01	0.42
2:B:2431:ASN:OD1	2:B:2431:ASN:N	2.52	0.42
2:B:2458:GLY:HA3	3:B:2901:ANP:H4'	2.01	0.42
2:A:1524:LYS:HZ1	2:A:1960:GLU:HA	1.84	0.42
2:A:2785:GLU:O	2:A:2788:VAL:HG12	2.19	0.42
2:B:1322:VAL:O	2:B:1326:VAL:HG23	2.19	0.42
2:B:2110:LEU:HD21	2:B:2123:TYR:CG	2.54	0.42
2:B:2459:ILE:CG2	2:B:2733:MET:CE	2.97	0.42
2:B:2659:LYS:HB3	2:B:2727:ARG:NE	2.34	0.42
2:A:1886:LEU:HD13	2:A:1892:ILE:HD12	2.01	0.42
2:A:1984:GLN:OE1	2:A:1984:GLN:N	2.52	0.42
2:B:2040:TYR:C	2:B:2044:LEU:HB2	2.44	0.42
2:B:2075:ASP:OD1	2:B:2076:LEU:N	2.52	0.42
2:A:372:PHE:H	2:A:382:GLU:H	1.68	0.42
2:A:1852:ASN:HD22	2:A:1857:ASN:HB2	1.83	0.42
2:A:2096:ARG:HE	2:A:2096:ARG:HB3	1.71	0.42
2:A:2666:VAL:HG23	2:A:2795:ALA:HA	2.02	0.42
2:B:1365:TYR:CE1	2:B:1630:ILE:HG23	2.54	0.42
2:B:1998:GLN:HG3	2:B:2505:SER:HA	2.02	0.42
2:B:2270:ARG:HA	2:B:2273:THR:HG22	2.01	0.42
2:B:2150:LEU:O	2:B:2153:MET:HB3	2.19	0.42
2:B:2290:HIS:O	2:B:2290:HIS:ND1	2.45	0.42
2:B:2479:VAL:HG22	2:B:2530:VAL:HG22	2.02	0.42
2:A:1531:PHE:HD2	2:A:1532:PRO:HD2	1.84	0.42
2:A:2071:TYR:CE2	2:A:2082:LYS:HB2	2.55	0.42
2:B:1455:PHE:H	2:B:1457:ARG:NH2	2.17	0.42
2:B:1661:ASN:O	2:B:1665:GLU:HG2	2.19	0.42
2:B:1993:LEU:HD22	2:B:2053:ILE:HG13	2.01	0.42
2:A:1810:LEU:HD12	2:A:1819:TYR:H	1.85	0.42
2:A:2131:TYR:OH	2:A:2175:ASN:HA	2.20	0.42
2:A:2364:LYS:HA	2:A:2367:LEU:HD12	2.00	0.42
2:A:678:SER:HA	2:A:1941:ASN:HD22	1.85	0.42
2:A:1803:ILE:HD13	2:A:1803:ILE:HA	1.88	0.42
2:B:2521:VAL:HG22	2:B:2531:ILE:HG22	2.02	0.42
2:A:578:GLN:C	2:A:580:SER:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1370:VAL:HG11	2:A:1394:HIS:CD2	2.55	0.42
2:A:1609:MET:O	2:A:1617:GLN:N	2.52	0.42
2:A:2110:LEU:HD21	2:A:2123:TYR:HA	2.01	0.42
2:A:2189:GLU:HG3	2:A:2236:TYR:HE1	1.85	0.42
2:A:2486:LEU:HA	2:A:2486:LEU:HD23	1.76	0.42
2:A:2576:ARG:HH21	2:B:2234:ARG:HH22	1.68	0.42
2:A:2787:SER:O	2:A:2790:GLU:HG3	2.20	0.42
2:B:1879:ASN:ND2	2:B:1902:SER:HB3	2.35	0.42
2:B:1965:LEU:HA	2:B:1968:TYR:HD2	1.85	0.42
2:B:2543:TYR:CE2	2:B:2594:PHE:HB2	2.55	0.42
2:B:2543:TYR:CG	2:B:2544:LEU:N	2.88	0.42
2:B:2708:VAL:O	2:B:2712:LEU:HD12	2.20	0.42
2:A:2403:ASP:HA	2:A:2454:HIS:CD2	2.55	0.41
2:B:2044:LEU:HD23	2:B:2044:LEU:HA	1.58	0.41
2:B:2373:ASN:O	2:B:2377:SER:N	2.53	0.41
2:A:98:ARG:O	2:A:102:ILE:N	2.51	0.41
2:A:1825:GLU:HG3	2:B:2108:GLU:OE1	2.20	0.41
2:B:1526:TYR:HB2	2:B:1528:ILE:HD11	2.02	0.41
2:B:1730:LEU:HD23	2:B:1730:LEU:HA	1.90	0.41
2:B:1819:TYR:HD1	2:B:1819:TYR:O	2.04	0.41
2:B:2141:VAL:O	2:B:2143:LYS:N	2.53	0.41
2:B:2165:TYR:CE1	2:B:2256:LYS:HD3	2.55	0.41
2:B:2612:TYR:OH	2:B:2674:VAL:HG13	2.20	0.41
2:A:2124:ALA:HB3	2:A:2164:ILE:HD12	2.02	0.41
2:A:2346:SER:OG	2:A:2347:ASN:N	2.52	0.41
2:A:2483:ASN:HA	2:A:2527:LYS:HA	2.02	0.41
2:A:2489:ASP:O	2:A:2493:GLU:HG2	2.20	0.41
2:B:1384:GLN:O	2:B:1387:GLY:N	2.53	0.41
2:B:1564:ASP:HB2	2:B:1565:PRO:HD3	2.01	0.41
2:B:2311:LEU:HD13	2:B:2362:ALA:HB3	2.01	0.41
2:B:2427:PRO:O	2:B:2430:MET:HG2	2.20	0.41
2:A:1284:ASN:HA	2:A:1430:ALA:HB1	2.02	0.41
2:A:1460:ILE:HD12	2:A:1460:ILE:HA	1.92	0.41
2:A:1483:ARG:H	2:A:1485:HIS:CE1	2.38	0.41
2:B:2459:ILE:HG22	2:B:2733:MET:HE3	2.01	0.41
2:A:1209:ILE:N	2:A:1210:PRO:HD2	2.34	0.41
2:A:1504:LEU:HD11	2:A:1515:LEU:HD13	2.01	0.41
2:A:1714:ASN:OD1	2:A:1714:ASN:N	2.51	0.41
2:A:2126:LEU:HB3	2:A:2145:TYR:HD2	1.85	0.41
2:A:2625:VAL:HG13	2:A:2774:VAL:HG13	2.03	0.41
2:A:2696:GLU:HG3	2:A:2697:THR:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1390:ILE:HA	2:B:1394:HIS:CE1	2.56	0.41
2:B:2310:ARG:NH1	2:B:2714:TYR:O	2.53	0.41
2:B:2457:SER:O	2:B:2458:GLY:C	2.61	0.41
2:A:1759:ASN:ND2	2:A:2551:TYR:HA	2.35	0.41
2:A:2286:ASN:O	2:A:2289:GLN:HG3	2.20	0.41
2:A:2543:TYR:C	2:A:2545:ASP:H	2.27	0.41
2:B:588:TRP:O	2:B:592:HIS:N	2.50	0.41
2:B:1715:ASN:OD1	2:B:1716:LYS:N	2.53	0.41
2:B:2790:GLU:HG2	2:B:2793:ARG:HH21	1.86	0.41
2:A:2435:ASN:ND2	2:A:2438:GLY:H	2.18	0.41
2:A:2632:HIS:CG	2:A:2633:GLY:N	2.89	0.41
2:B:1662:TRP:O	2:B:1666:GLU:HG3	2.20	0.41
2:B:2572:ASP:O	2:B:2576:ARG:HG2	2.21	0.41
2:A:1427:LYS:HE2	2:A:1431:ILE:HD11	2.03	0.41
2:A:1560:ILE:HG23	2:A:1561:PRO:O	2.21	0.41
2:A:1580:ILE:HD12	2:A:1580:ILE:H	1.86	0.41
2:A:1599:LEU:HD13	2:A:1693:PHE:HE2	1.86	0.41
2:A:1686:LEU:O	2:A:1689:TYR:HB3	2.21	0.41
2:A:2243:ARG:O	2:A:2246:MET:HG2	2.20	0.41
2:A:2425:LEU:HD23	2:A:2425:LEU:HA	1.93	0.41
2:B:523:LEU:O	2:B:527:ASN:N	2.51	0.41
2:B:1417:LEU:HD12	2:B:1417:LEU:O	2.21	0.41
2:B:1441:TYR:O	2:B:1445:LEU:HG	2.20	0.41
2:B:1521:LYS:HE3	2:B:1521:LYS:HB2	1.91	0.41
2:B:2254:TYR:O	2:B:2258:LEU:HG	2.21	0.41
2:B:2311:LEU:O	2:B:2359:ARG:HG2	2.21	0.41
2:A:1532:PRO:HD2	2:A:1535:LEU:HB3	2.02	0.41
2:A:1605:ASP:HA	2:A:1608:ARG:HB3	2.02	0.41
2:A:1949:ILE:HG13	2:A:1974:LEU:HD22	2.03	0.41
2:A:2022:GLN:OE1	2:A:2037:ARG:HB2	2.21	0.41
2:A:2626:LEU:HD23	2:A:2654:PHE:HE1	1.86	0.41
2:B:211:ARG:O	2:B:215:GLN:N	2.53	0.41
2:B:1066:ILE:N	2:B:1102:LYS:O	2.53	0.41
2:B:1182:ILE:HD13	2:B:1208:LEU:HD23	2.03	0.41
2:B:1387:GLY:HA2	2:B:1390:ILE:HD12	2.02	0.41
2:B:1512:LEU:HD23	2:B:1512:LEU:HA	1.89	0.41
2:B:1547:PHE:CG	2:B:1965:LEU:HD21	2.55	0.41
2:B:1647:GLN:H	2:B:1650:LYS:HB2	1.85	0.41
2:B:1690:MET:O	2:B:1694:SER:N	2.48	0.41
2:B:1841:SER:N	2:B:1842:PRO:HD2	2.36	0.41
2:A:1397:LYS:HA	2:A:1397:LYS:HD3	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2009:LEU:CD2	2:A:2013:ILE:HD11	2.51	0.41
2:A:2292:LEU:HD13	2:A:2325:ILE:HD11	2.03	0.41
2:A:2307:LEU:HD12	2:A:2307:LEU:HA	1.88	0.41
2:A:2480:LYS:HZ1	2:A:2531:ILE:HD11	1.85	0.41
2:A:2487:ARG:HD3	2:A:2717:LEU:HD22	2.03	0.41
2:B:1284:ASN:ND2	2:B:1388:LEU:HD13	2.35	0.41
2:A:1330:LEU:HD11	2:A:1350:LEU:HD23	2.02	0.40
2:A:1564:ASP:HB2	2:A:1579:ILE:HG21	2.02	0.40
2:A:1680:THR:O	2:A:1684:LYS:HG2	2.21	0.40
2:A:2185:PHE:CE2	2:A:2243:ARG:HD3	2.55	0.40
2:A:2227:SER:O	2:A:2231:ILE:HG12	2.21	0.40
2:A:2333:HIS:HE1	2:A:2440:TYR:HE2	1.68	0.40
2:B:325:LEU:CB	2:B:394:ILE:HA	2.52	0.40
2:B:1475:GLU:HA	2:B:1478:ASN:HD21	1.86	0.40
2:B:2600:ALA:HB3	2:B:2604:GLN:HB3	2.03	0.40
2:B:2710:GLU:O	2:B:2714:TYR:HD2	2.05	0.40
2:A:1523:TYR:OH	2:A:1965:LEU:HB2	2.22	0.40
2:A:1548:PHE:CE1	2:A:1969:ALA:HB1	2.56	0.40
2:A:1919:LYS:HA	2:A:1919:LYS:HD3	1.78	0.40
2:A:2705:LEU:HD12	2:A:2705:LEU:HA	1.64	0.40
2:B:1685:LEU:HD12	2:B:1686:LEU:N	2.36	0.40
2:B:2137:LYS:HE3	2:B:2139:GLU:HB3	2.03	0.40
2:B:2595:PHE:C	2:B:2605:TRP:HD1	2.29	0.40
2:A:625:ARG:N	2:A:1944:HIS:HB2	2.35	0.40
2:A:1065:SER:C	2:A:1103:LEU:HA	2.46	0.40
2:A:1751:ARG:HD2	2:A:1751:ARG:HA	1.79	0.40
2:A:2002:GLN:O	2:A:2003:LEU:HB2	2.22	0.40
2:A:2394:ALA:HB2	2:A:2479:VAL:HB	2.04	0.40
2:A:2698:LEU:HD13	2:A:2698:LEU:HA	1.89	0.40
2:B:1245:SER:HA	2:B:1248:PHE:CD1	2.57	0.40
2:B:2022:GLN:NE2	2:B:2037:ARG:HG2	2.37	0.40
1:F:71:LEU:O	1:F:71:LEU:HD12	2.20	0.40
2:A:1533:ASP:OD1	2:A:1534:SER:N	2.55	0.40
2:A:1607:ILE:O	2:A:1610:PHE:HB2	2.22	0.40
2:A:2428:ILE:H	2:A:2428:ILE:HG13	1.68	0.40
2:A:2623:GLY:O	2:A:2627:GLY:N	2.54	0.40
2:A:2654:PHE:HD2	2:A:2720:TRP:HD1	1.69	0.40
2:B:1361:ILE:HA	2:B:1366:LEU:CD2	2.51	0.40
2:B:1651:LEU:HD12	2:B:1651:LEU:HA	1.92	0.40
2:B:2595:PHE:N	2:B:2595:PHE:CD1	2.90	0.40
2:B:2784:VAL:O	2:B:2788:VAL:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1750:ARG:HH22	2:A:2597:GLU:H	1.68	0.40
2:A:1946:GLU:HG3	2:A:1979:ARG:NH1	2.37	0.40
2:A:1974:LEU:HG	2:A:2017:LEU:HD21	2.04	0.40
2:A:2256:LYS:HB2	2:A:2256:LYS:HE2	1.81	0.40
2:A:2342:PHE:O	2:A:2346:SER:N	2.54	0.40
2:A:2352:GLU:OE2	2:A:2352:GLU:N	2.36	0.40
2:A:2568:LYS:HZ3	2:A:2580:TYR:HB2	1.86	0.40
2:A:2606:PHE:CD1	2:A:2606:PHE:C	2.99	0.40
2:B:2089:SER:O	2:B:2093:LEU:HG	2.22	0.40
2:B:2165:TYR:HB3	2:B:2253:HIS:O	2.22	0.40
2:B:2188:MET:HE3	2:B:2192:TYR:HB2	2.03	0.40
2:B:2244:SER:OG	2:B:2283:GLU:OE2	2.37	0.40
2:B:2245:LYS:O	2:B:2249:GLN:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
2	A	2372/2812 (84%)	2222 (94%)	142 (6%)	8 (0%)	37	66
2	B	2330/2812 (83%)	2190 (94%)	137 (6%)	3 (0%)	48	78
All	All	4708/5632 (84%)	4417 (94%)	280 (6%)	11 (0%)	45	72

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	1571	LYS
2	A	2640	LYS
2	A	2658	LYS
2	A	2462	PRO

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Mol	Chain	Res	Type
2	A	2562	ARG
2	A	2410	PHE
2	A	355	VAL
2	B	355	VAL
2	A	576	VAL
2	B	546	ILE
2	B	576	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	8/8 (100%)	8 (100%)	0	100	100
2	A	1106/2621 (42%)	1090 (99%)	16 (1%)	62	78
2	B	1126/2621 (43%)	1113 (99%)	13 (1%)	67	80
All	All	2240/5250 (43%)	2211 (99%)	29 (1%)	64	79

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	1470	LYS
2	A	1791	LEU
2	A	1935	ASN
2	A	1970	LEU
2	A	2005	GLU
2	A	2068	ASP
2	A	2341	LEU
2	A	2348	VAL
2	A	2459	ILE
2	A	2548	HIS
2	A	2564	LEU
2	A	2637	LEU
2	A	2658	LYS
2	A	2659	LYS
2	A	2660	LEU

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Mol	Chain	Res	Type
2	A	2665	CYS
2	B	1456	LEU
2	B	1599	LEU
2	B	1634	SER
2	B	1766	TRP
2	B	2457	SER
2	B	2460	ASN
2	B	2485	ASP
2	B	2723	SER
2	B	2726	ARG
2	B	2728	MET
2	B	2729	LYS
2	B	2730	LYS
2	B	2732	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	1703	HIS
2	A	1744	ASN
2	A	1752	GLN
2	A	1852	ASN
2	A	1935	ASN
2	A	2286	ASN
2	A	2332	ASN
2	A	2333	HIS
2	A	2454	HIS
2	A	2477	GLN
2	A	2494	GLN
2	A	2511	GLN
2	B	1289	ASN
2	B	1558	HIS
2	B	1744	ASN
2	B	1759	ASN
2	B	1879	ASN
2	B	1957	ASN
2	B	1996	ASN
2	B	2128	ASN
2	B	2152	HIS
2	B	2374	GLN
2	B	2454	HIS
2	B	2477	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	ANP	A	2901	-	29,33,33	1.09	4 (13%)	31,52,52	1.10	2 (6%)
3	ANP	B	2901	-	29,33,33	1.09	4 (13%)	31,52,52	1.05	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	A	2901	-	-	5/14/38/38	0/3/3/3
3	ANP	B	2901	-	-	7/14/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2901	ANP	PG-N3B	2.47	1.69	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2901	ANP	PG-O1G	2.45	1.50	1.46
3	A	2901	ANP	PG-N3B	2.44	1.69	1.63
3	A	2901	ANP	PG-O1G	2.39	1.49	1.46
3	A	2901	ANP	PB-O3A	-2.36	1.56	1.59
3	B	2901	ANP	PB-O3A	-2.29	1.56	1.59
3	A	2901	ANP	PB-O1B	2.28	1.49	1.46
3	B	2901	ANP	PB-O1B	2.23	1.49	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2901	ANP	PB-O3A-PA	-3.84	119.09	132.62
3	B	2901	ANP	PB-O3A-PA	-3.61	119.91	132.62
3	A	2901	ANP	C5-C6-N6	2.29	123.83	120.35
3	B	2901	ANP	C5-C6-N6	2.28	123.81	120.35

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2901	ANP	PB-N3B-PG-O1G
3	A	2901	ANP	O4'-C4'-C5'-O5'
3	B	2901	ANP	PB-N3B-PG-O1G
3	B	2901	ANP	C5'-O5'-PA-O3A
3	A	2901	ANP	C3'-C4'-C5'-O5'
3	B	2901	ANP	O4'-C4'-C5'-O5'
3	A	2901	ANP	C4'-C5'-O5'-PA
3	B	2901	ANP	C4'-C5'-O5'-PA
3	B	2901	ANP	C5'-O5'-PA-O1A
3	B	2901	ANP	PG-N3B-PB-O3A
3	B	2901	ANP	C3'-C4'-C5'-O5'
3	A	2901	ANP	C5'-O5'-PA-O1A

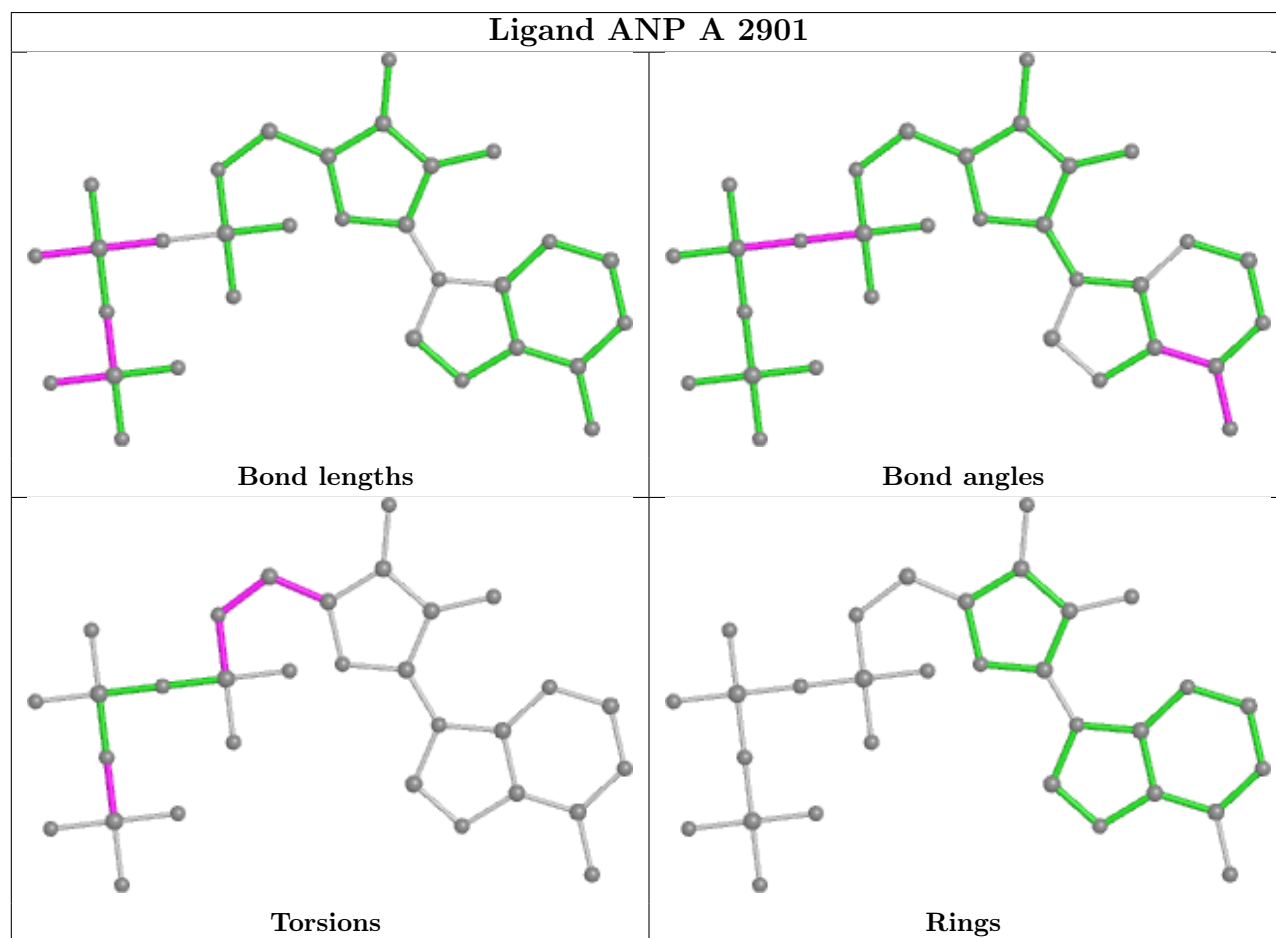
There are no ring outliers.

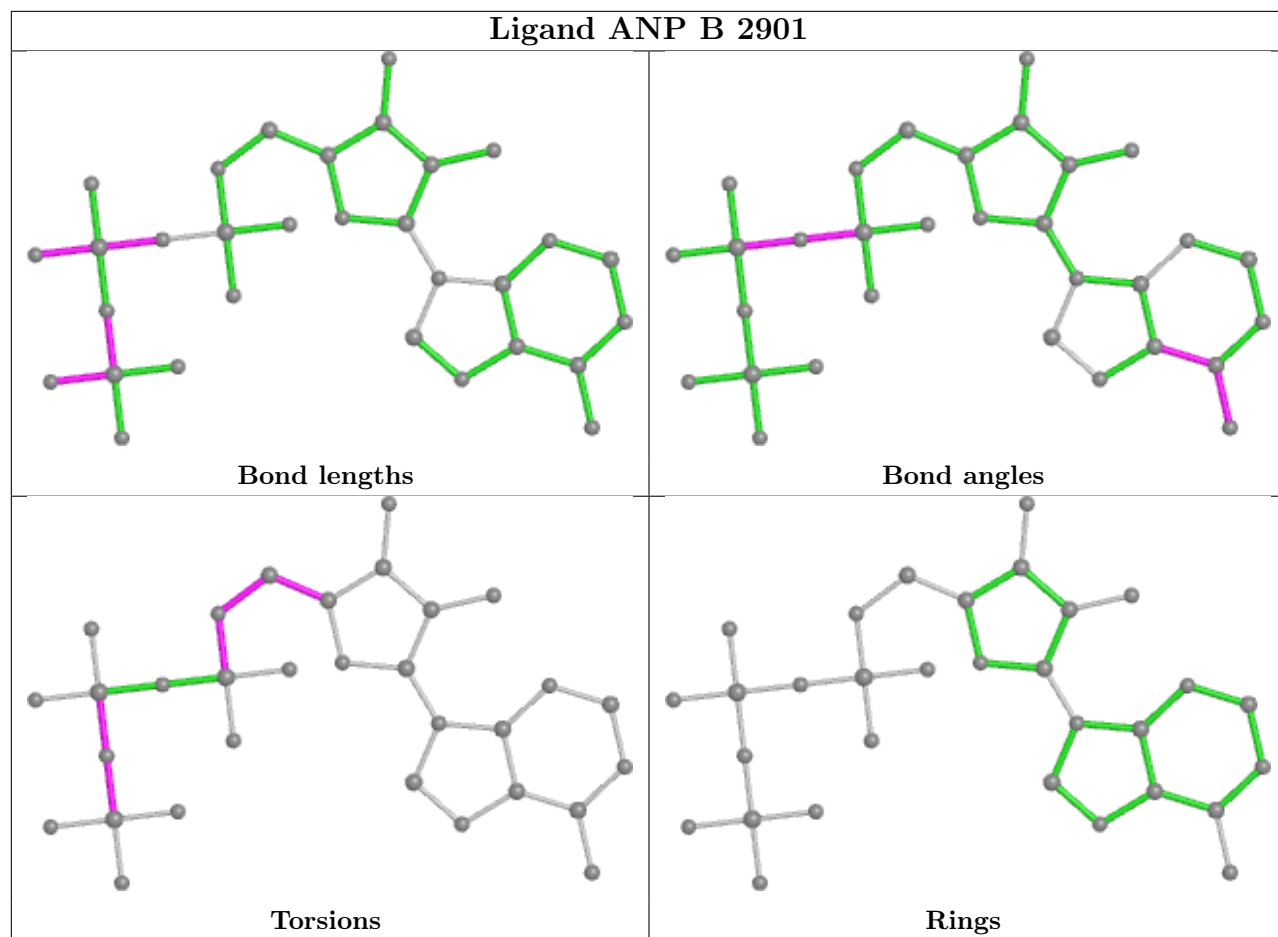
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2901	ANP	3	0
3	B	2901	ANP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.